Component-based model order reduction procedure for large scales Thermo-Hydro-Mechanical systems

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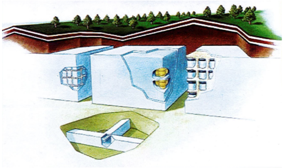
Motivations

Management of radioactive waste materials.
Solution by *Andra*[1]:

- deep-depth repository ($300 - 500\,m$) in geological media
- long term isolation



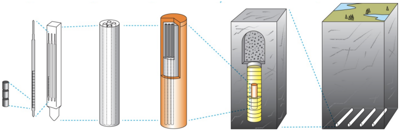
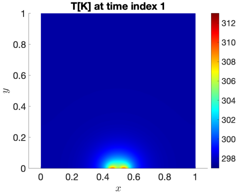


Figure 1: Packages of radioactive waste in repository structures (*alveoli*).

[1] French National Agency for radioactive waste management.

The THM model

- High temperature radioactive waste
- Hydro-mechanical response of the geological medium



The problem is described by **Thermo-Hydro-Mechanical** (**THM**) systems of PDEs:

- **mechanics**: linear elasticity
- **hydraulics**: water mass conservation law, Darcy's law
- **heat transfer**: energy conservation, heat conduction

The THM model

- **State variables** $\underline{U} = [\underline{u}^{\mathrm{T}}, p_{\mathrm{w}}, T]^{\mathrm{T}}$;
- **Internal variables** $\underline{W} = [\rho_{\mathrm{w}}, \varphi, h_{\mathrm{w}}, Q, \underline{M}_{\mathrm{w}}^{\mathrm{T}}, m_{\mathrm{w}}]^{\mathrm{T}}$.

Given $\mu \in \mathcal{P}$, find $\underline{U}_\mu$ and $\underline{W}_\mu$ such that

$$\begin{cases} \mathcal{G}_\mu(\underline{U}_\mu, \partial_t \underline{U}_\mu, \underline{W}_\mu) = 0, & \text{in } \Omega \times (0, T_{\mathrm{f}}], \\ \dot{\underline{W}}_\mu = \mathcal{F}_\mu(\underline{U}_\mu, \underline{W}_\mu), & \text{in } \Omega \times (0, T_{\mathrm{f}}], \end{cases}$$

with $\underline{U}_\mu(\cdot, 0) = \underline{U}_0$, $\underline{W}_\mu(\cdot, 0) = \underline{W}_0$.

Challenges of the numerical model:

high nonlinearity, time dependency, high dimensionality

The THM system

Parametrized system:

- geometric configuration (e.g. the number of the alveoli);
- material properties of the medium.

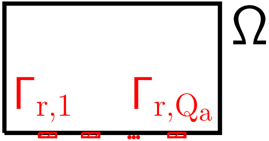


Figure 2: Domain Ω and boundaries $\Gamma_{\mathrm{r},1}, \ldots, \Gamma_{\mathrm{r},Q_\mathrm{a}}$.

Challenges

- uncertainty in the parameters: **multi-query** and almost **real-time** context
- geometric parameters cause **topology changes**

Objective and contributions

Objective

develop a **component-based (CB) model order reduction (MOR)** procedure for **parametrized problems** in nonlinear mechanics, with emphasis on **THM systems**.

1. Design of a **monolithic MOR** technique for THM systems [2]
2. Design of a **CB-pMOR** formulation for parametrized nonlinear (steady) elliptic PDEs. [3]
3. Extension of the **CB-pMOR** formulation to THM systems.

[2] Iollo, Sambataro, Taddei, *IJNME*, 2022.
[3] Iollo, Sambataro, Taddei, *CMAME*, 2023.

Outline of the presentation

1. A **monolithic model reduction** method for THM systems
2. **CB-pMOR** methodology for steady problems: application to a nonlinear elasticity problem
3. **CB-pMOR** methodology for time-dependent problems with internal variables: application to the THM problem.
4. Conclusions and perspectives

Time-marching Galerkin ROM

The Reduced Basis method

Methodology: given a Hilbert space $(\mathcal{X}, \|\cdot\|)$ over $\Omega \subset \mathbb{R}^d$ and the parametric set $\mathcal{P} \subset \mathbb{R}^{\mathrm{P}}$, $P \geq 1$,

for each $\mu \in \mathcal{P}$ and each time index $j = 1, \ldots, J_{\max}$ we seek

$$\underline{\hat{U}}_{\mu}^{(j)} = \underline{Z}_N \alpha_{\mu}^{(j)} = \sum_{n=1}^{N} \left(\alpha_{\mu}^{(j)}\right)_n \underline{\zeta}_n$$

where

- **reduced coefficients** $\alpha_{\mu}^{(j)} : \mathcal{P} \to \mathbb{R}^N$;
- **reduced order basis (ROB)** $\underline{Z}_N : \mathbb{R}^N \to \mathcal{Z}_N$ s.t. $\mathcal{Z}_N = \mathrm{span}\{\underline{\zeta}_n\}_{n=1}^N \subset \mathcal{X}^{\mathrm{hf}}$.

Time-marching Galerkin ROM

The Reduced Basis method

Rationale: we approximate the solution manifold

$$\mathcal{M} = \{\underline{U}_\mu^{(j)} \in \mathcal{X}^{\mathrm{hf}} : \mu \in \mathcal{P}, j \in \{1, \ldots, J_{\max}\}\} \subset \mathcal{X}^{\mathrm{hf}},$$

by a **low-dimensional** linear space $\mathcal{Z}_N$, with $N \ll N^{\mathrm{hf}}$.

Linear compressibility is guaranteed by exponential decay of the *Kolmogorov n-width* for a wide range of elliptic and parabolic problems.

Offline/online decomposition

Algorithm 1 Offline/online decomposition

Offline stage:

1: Define a properly selected training set Ξ_{train} and compute $\{\underline{U}_{\mu}^{(j)}\}_{j \in \mathrm{I_s}}$, $\mathrm{I_s} \subset \{1, \dots, J_{\max}\}$ $\forall\, \mu \in \Xi_{\mathrm{train}}$

2: construct the ROB $Z_N : \mathbb{R}^N \to \mathcal{Z}_N$ ▷ **data compression**

3: construct the ROM with hyper-reduction structures. ▷ **hyper-reduction**

Online stage:

4: Given $\mu \in \Xi_{\mathrm{test}}$, compute $\{\widehat{\boldsymbol{\alpha}}_{\mu}^{(k)}\}_{j=1}^{J_{\max}}$ by solving the ROM

ROM=reduced order model

Construction of the reduced space

Two challenges:

1. sampling of $\mathcal{P}$,
2. compression strategy.

For time-dependent problems: **POD-Greedy method:**[4]

- **Greedy search** driven by an *error indicator*
- **POD**-based **data compression**: find small orthonormal basis that is optimal in the $L^2(\Xi_{\mathrm{train}})$ sense:

$$\mathcal{Z}_n = \arg \inf_{\mathcal{Z}\subset\mathcal{X}, \dim\mathcal{Z}=\mathrm{n}} \frac{1}{n_{\mathrm{train}}} \sum_{k=1}^{n_{\mathrm{train}}} \|\underline{U}_k - \Pi_{\mathcal{Z}} \underline{U}_k\|^2$$

$$\text{where } \Pi_{\mathcal{Z}_n}(\underline{U}_\mu^{(j)}) = \arg \min_{\underline{V}\in\mathcal{Z}_n} \|\underline{U}_\mu^{(j)} - \underline{V}\|$$

[4] Haasdonk, Ohlberger, M2AN, 2008; Haasdonk, ESAIM, 2013.

POD-Greedy algorithm

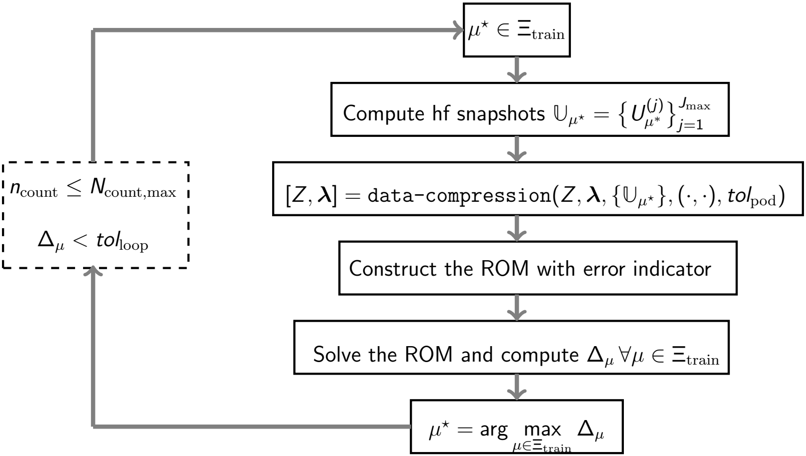


Figure 3: Adaptive algorithm based on POD-Greedy procedure

Data compression

Motivation: constrained memory capacities of standard POD:

$$[\mathbf{Z},\ \boldsymbol{\lambda}] \leftarrow \texttt{POD}\left(\{\mathbb{U}_k\}_{k=1}^{n_{\mathrm{train}}}, (\cdot,\cdot), tol_{\mathrm{pod}}\right).$$

Given $\mathbf{Z}$ and the snapshots $\mathbb{U}_{\mu^\star}$,

- **hierarchical POD (HPOD)**[5]

$$\mathbf{Z}' = [\mathbf{Z}, \mathbf{Z}^{\mathrm{new}}],\ \mathbf{Z}^{\mathrm{new}} \leftarrow \texttt{POD}\left(\left\{\Pi_{\mathcal{Z}^{orth}}\mathbb{U}_{\mu^\star}\right\}_k, (\cdot,\cdot), tol_{\mathrm{pod}}\right),$$

- **hierarchical approximate POD (HAPOD)**[6]

$$[\mathbf{Z}', \boldsymbol{\lambda}'] \leftarrow \texttt{POD}\left(\left\{\mathbb{U}_{\mu^\star}\right\} \cup \left\{\sqrt{\lambda_N}\,\zeta_N\right\}_{N=1}^{n}, (\cdot,\cdot), tol_{\mathrm{pod}}\right)$$

[5] Haasdonk, SIAM 2017.

[6] Himpe, Leibner, Rave, SIAM, 2018.

Reduced formulation

- **Galerkin projection**

$$\begin{cases} \mathcal{G}_\mu^{\mathrm{hf}}\left(\widehat{\mathbf{U}}_\mu^{(j)},\, \mathbf{U}_\mu^{(j-1)},\, \mathbf{W}_\mu^{(j)},\, \mathbf{W}_\mu^{(j-1)},\, \mathbf{V}\right) = 0,\ \forall\, \underline{V} \in \mathcal{Z}_N \\ \mathbf{W}_\mu^{(j)} = \mathcal{F}_\mu^{\mathrm{hf}}(\mathbf{U}_\mu^{(j)}, \mathbf{U}_\mu^{(j-1)}, \mathbf{W}_\mu^{(j-1)}) \end{cases}$$

System of N equations to be solved, for $N \ll N^{\mathrm{hf}}$.

- Alternative reduced formulation: **minimum residual formulation**. [7]

[7] Farhat et al, JCP, 2013.

Galerkin ROM

Computational bottleneck: integration over the full mesh; **proposed solution:** integration on a **reduced mesh**.

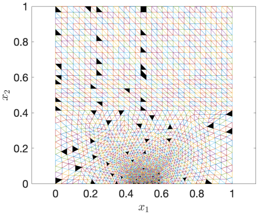
High-fidelity residual:

$$\mathcal{R}^{\rm hf}_{\mu}\left(\mathbb{U}_{\mu}, \mathbf{V}\right) = \sum_{k=1}^{N_{\rm e}} r^{\rm hf}_{\mu,k}\left(\mathbf{E}_k \mathbf{U}_{\mu}^{(j)}, \mathbf{E}_k \mathbf{U}_{\mu}^{(j-1)}, \left(\mathbf{W}_{\mu}^{(j)}\right)_{\cdot,k,\cdot}, \left(\mathbf{W}_{\mu}^{(j-1)}\right)_{\cdot,k,\cdot}, \mathbf{E}_k \mathbf{V}_{\cdot}\right)$$

Empirical quadrature residual:

$$\mathcal{R}^{\rm eq}_{\mu}\left(\hat{\mathbb{U}}_{\mu}, \mathbf{V}\right) = \sum_{k \in \mathtt{I}_{\rm eq}} \rho^{\rm eq}_k \, r^{\rm hf}_{\mu,k}\left(\cdot, \cdot, \cdot, \cdot, \cdot\right)$$

where $\boldsymbol{\rho}^{\rm eq} = [\rho^{\rm eq}_1, \ldots, \rho^{\rm eq}_{N_{\rm e}}]^T$ s.t. $\rho^{\rm eq}_k = 0$ if $k \notin \mathtt{I}_{\rm eq}$, $\boldsymbol{\rho}^{\rm eq} \geq \mathbf{0}$.



Question: choice of $\boldsymbol{\rho}^{\rm eq}$.

Hyper-reduction

EQ procedure

Find $\boldsymbol{\rho}^{\mathrm{eq}} \in \mathbb{R}^{\mathrm{e}}$ s.t.

1. $\|\boldsymbol{\rho}^{\mathrm{eq}}\|_0$ is as small as possible;
2. the entries of $\boldsymbol{\rho}^{\mathrm{eq}}$ are non-negative;
3. *constant-function constraint*: [8]

$$\left| \sum_{k=1}^{N_{\mathrm{e}}} \rho_k^{\mathrm{eq}} |\mathtt{D}_k| - |\Omega| \right| \ll 1;$$

4. *manifold accuracy constraint*:

$$\left\| \left(\mathbf{J}_{\mu}^{\mathrm{hf}} \left(\boldsymbol{\alpha}_{\mathrm{train}}^{(j)} \right) \right)^{-1} \left(\widehat{\mathbf{R}}_{\mu}^{\mathrm{hf}} \left(\boldsymbol{\alpha}_{\mathrm{train}}^{(j)} \right) - \widehat{\mathbf{R}}_{\mu}^{\mathrm{eq}} \left(\boldsymbol{\alpha}_{\mathrm{train}}^{(j)} \right) \right) \right\|_2 \ll 1.$$

[8] Farhat et al, IJNME, 2015; Yano, Patera, CMAME, 2019; Ryckelynck, IJNME, 2009.

Hyper-reduction

Sparse representation problem (NP-hard)[9]

$$\text{find } \boldsymbol{\rho}^{\text{eq}} \in \arg\min_{\boldsymbol{\rho}\in\mathbb{R}^{\mathrm{N_e}}} \|\boldsymbol{\rho}\|_0 \,\text{s.t.} \begin{cases} \boldsymbol{\rho} \geq \mathbf{0} \\ \|\mathbf{C}\boldsymbol{\rho} - \mathbf{b}\|_* \leq \delta, \end{cases}$$

for a suitable choices of the matrix $\mathbf{C}$, the vector $\mathbf{b}$, the norm $\|\cdot\|_*$, and the tolerance δ.

Inexact non-negative least squares (NNLS) problem

$$\min_{\boldsymbol{\rho}\in\mathbb{R}^{N_e}} \|\mathbf{C}\boldsymbol{\rho} - \mathbf{b}\|_2 \,\text{s.t.}\, \boldsymbol{\rho} \geq \mathbf{0}.$$

[9] Lawson CL, Hanson RJ, SIAM 1974; Farhat et al, IJNME, 2015.

Error indicator

Goal: find an inexpensive and accurate indicator of the true error

$$E_\mu := \frac{\sqrt{\sum_{j=1}^{J_{\max}} \left(t^{(j)} - t^{(j-1)}\right) \left\| \underline{U}_\mu^{(j)} - \underline{\widehat{U}}_\mu^{(j)} \right\|^2}}{\sqrt{\sum_{j=1}^{J_{\max}} \left(t^{(j)} - t^{(j-1)}\right) \left\| \underline{U}_\mu^{(j)} \right\|^2}}$$

First proposal: time-discrete $L^2(0, T_\mathrm{f}; \mathcal{Y}')$ residual indicator [10]

$$\Delta_\mu^{\mathrm{hf}}(\mathbb{U}) = \sqrt{\sum_{j=1}^{J_{\max}} \left(t^{(j)} - t^{(j-1)}\right) \left(\sup_{\underline{V} \in \mathcal{Y} \setminus \{0\}} \frac{\mathcal{R}_\mu^{\mathrm{hf}}(\underline{U}^{(j)}, \underline{V})}{\|\underline{V}\|_{\mathcal{Y}}} \right)^2}.$$

[10] Haasdonk, Ohlberger, M2AN, 2008.

Error indicator

Our proposal: time-average hyper-reduced error indicator [11]

$$\Delta_\mu(\mathbb{U}_\mu, \mathbb{W}_\mu) = \sup_{\underline{V} \in \mathcal{Y}_M \setminus \{0\}} \frac{\mathcal{R}^{\mathrm{eq,r}}_{\mathrm{avg},\mu}(\mathbb{U}_\mu, \mathbb{W}_\mu, \underline{V})}{\|\underline{V}\|},$$

where

$$\mathcal{R}^{\mathrm{eq}}_{\mathrm{avg},\mu}(\mathbb{U}_\mu, \mathbb{W}_\mu, \underline{V}) := \sum_{j=1}^{J_{\max}} (t^{(j)} - t^{(j-1)}) \mathcal{R}^{\mathrm{eq}}_\mu(\underline{U}^{(j)}_\mu, \underline{U}^{(j-1)}_\mu, \underline{W}^{(j)}_\mu, \underline{W}^{(j-1)}_\mu, \underline{V})$$

[11] Fick et al, JCP, 2018.

Numerical setting

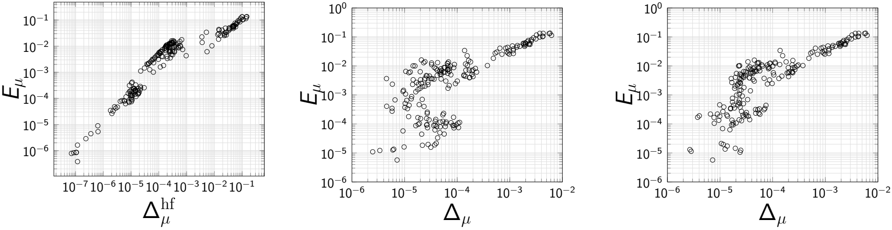
The THM problem

- **Newton's method** with line-search;
- **Implicit Euler** time discretization, with $J_{\max} = 100$ uniform time steps;
- $\mathrm{p} = 3$ FE discretization for the displacement, $\mathrm{p} = 2$ for pressure and temperature.

Parametrization: Young's modulus E, Poisson's ratio ν in the region UA, thermic factor τ and the constant C_{al}.

$$(E_1, \nu_1, \tau, C_{\mathrm{al}}) \overset{\mathrm{iid}}{\sim} \mathcal{U}\big([857.52, 1.16 \cdot 10^3] \times [0.25, 0.35] \\ \times [4.53, 6.13] \times [0.39, 0.52]\big)$$

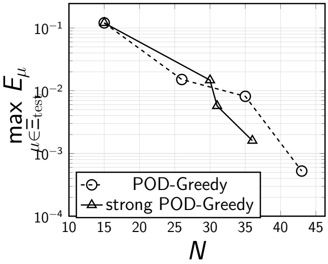
Error estimation



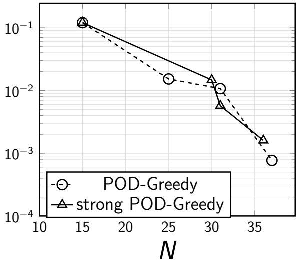
(a) H-POD (b) H-POD (c) HA-POD

Figure 4: correlation between the time-discrete $L^2(0, T_\mathrm{f}; \mathcal{Y}')$ with respect to the true relative error E_μ. (a):$L^2(0, T_\mathrm{f}; \mathcal{Y}')$, (b),(c):Δ_μ.

Prediction tests



(a) H-POD Greedy



(b) HA-POD Greedy

Figure 5: parametric problem:out-of-sample performance of the ROM parametric problem obtained using the POD-Greedy algorithm. Comparison with strong POD Greedy.

1. **A monolithic model reduction method for the THM problem**
   - Methodology
   - Numerical results

2. **A one-shot overlapping Schwarz method for CB-pMOR**
   - A one shot overlapping Schwarz formulation
   - CB-pMOR methodology
   - Numerical results

3. **A one-shot overlapping Schwarz method for the THM system**
   - Numerical results

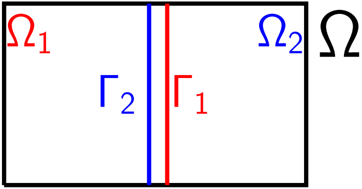
4. **Conclusions and perspectives**

Foundations of the method

We consider a steady problem of the type

$$\text{find } u_\mu \in \mathcal{X} : \mathcal{G}_\mu(u_\mu, v) = 0 \ \ \forall v \in \mathcal{Y},$$

with (or without) Dirichlet boundary conditions on a portion of the domain $\Gamma_{\mathrm{dir}} \subset \partial\Omega$. If $\mathcal{X} = H^1$, the test space $\mathcal{Y}$ is set equal to $H^1_{\Gamma_{\mathrm{dir}},0}$.



Foundations of the method

Let us consider the **Overlapping Schwarz** method

$$\begin{cases} \text{find } u_1^{(k)} \in \mathcal{X}_1 \,:\, \mathcal{G}_1(u_1^{(k)}, v) = 0 \;\; \forall\, v \in \mathcal{X}_{1,0}, \;\; u_1^{(k)}|_{\Gamma_1} = u_2^{(k-1)}; \\ \text{find } u_2^{(k)} \in \mathcal{X}_2 \,:\, \mathcal{G}_2(u_2^{(k)}, v) = 0 \;\; \forall\, v \in \mathcal{X}_{2,0}, \;\; u_2^{(k)}|_{\Gamma_2} = \begin{cases} u_1^{(k)} \\ u_1^{(k-1)} \end{cases}, \end{cases}$$

where $\mathcal{X}_{i,0} = \{v \in \mathcal{X}_i : v|_{\Gamma_i} = 0\}$.

Convergence of the OS iterations to a limit state $(u_1^\star, u_2^\star)$ implies that $\|u_1^\star - u_2^\star\|_{L^2(\Gamma_1 \cup \Gamma_2)} = 0$.

Proposal: one-shot overlapping Schwarz (OS2) method

MOR constrained optimization formulation

CB full-order model

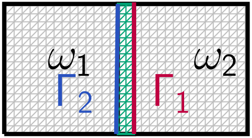
Given $\mu = (\mu_1, \mu_2) \in \mathcal{P} = \bigotimes_{i=1}^{2} \mathcal{P}^i$, find $u^{\mathrm{hf}} = (u_1, u_2) \in \mathcal{X} := \bigotimes_{i=1}^{2} \mathcal{X}_i$ to minimize

OS2 constrained optimization statement

$$\min_{u \in \mathcal{X}} \frac{1}{2} \left(\|u_1 - u_2\|^2_{L^2(\Gamma_1)} + \|u_2 - u_1\|^2_{L^2(\Gamma_2)} \right)$$

s.t.

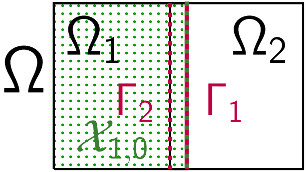
$$\mathcal{G}_1(u_1, v_1) = 0 \;\; \forall\, v_1 \in \mathcal{X}_{1,0},$$
$$\mathcal{G}_2(u_2, v_2) = 0 \;\; \forall\, v_2 \in \mathcal{X}_{2,0}$$



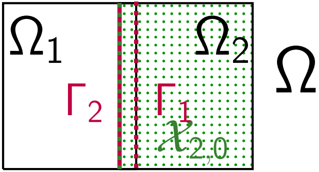
Solution decomposition

For $i = 1, 2$, given instantiated spaces $\mathcal{X}_i \subset [H^1_{0,\Gamma_i^{\mathrm{dir}}}]^D$,

- **Port space** $\mathcal{U}_i = \{v|_{\Gamma_i} : v \in \mathcal{X}_i\} \subset [H^{1/2}(\Gamma_i)]^D$
- **Bubble space** $\mathcal{X}_{i,0} = \{v \in \mathcal{X}_i : v|_{\Gamma_i} = 0\}$



(a) port and bubble spaces for $i = 1$



(b) port and bubble spaces for $i = 2$

Figure 6: Sketch of bubble and port nodes associated with (a):$\mathcal{X}_{1,0}$, Γ_1 and (b):$\mathcal{X}_{2,0}$, Γ_2.

Solution decomposition

Given $w \in \mathcal{U}_i$ and continuous extension operator $\mathtt{E}_i : \mathcal{U}_i \to \mathcal{X}_i$,

$$u_i = \underbrace{\boxed{\mathtt{F}_i(w)}}_{\textbf{bubble}} + \underbrace{\boxed{\mathtt{E}_i w}}_{\textbf{port}}$$

where $\mathtt{E}_i : \mathcal{U}_i \to \mathcal{X}_{i,0}$ is the **continuous extension operator**:

$$(\mathtt{E}_i w, v) = 0 \, \forall v \in \mathcal{X}_{i,0}, \quad \mathtt{E}_i w|_{\Gamma_i} = w;$$

$\mathtt{F}_i : \mathcal{U}_i \to \mathcal{X}_{i,0}$ is the **port-to-bubble maps.**

The variational forms $\mathcal{G}_i : \mathcal{X}_i \times \mathcal{X}_{i,0} \to \mathbb{R}$ satisfy [12]

$$\mathcal{G}_i \left(\mathtt{F}_i(w) + \mathtt{E}_i w, v \right) = 0 \quad \forall \, v \in \mathcal{X}_{i,0}.$$

[12] Huynh et al, ESAIM, 2013.

CB full-order model

Find $u^{\mathrm{hf,p}} = \left(u_1^{\mathrm{hf,p}}, u_2^{\mathrm{hf,p}}\right) \in \mathcal{U} := \bigotimes_{i=1}^{2} \mathcal{U}_i$ to minimize

Unconstrained optimization statement

$$\min_{u^{\mathrm{p}} \in \mathcal{U}} \frac{1}{2}\Big(\|\mathrm{E}_1 u_1^{\mathrm{p}} + \mathrm{F}_1(u_1^{\mathrm{p}}) - \mathrm{E}_2 u_2^{\mathrm{p}} - \mathrm{F}_2(u_2^{\mathrm{p}})\|^2_{L^2(\Gamma_1)} + \\ \|\mathrm{E}_2 u_2^{\mathrm{p}} + \mathrm{F}_2(u_2^{\mathrm{p}}) - \mathrm{E}_1 u_1^{\mathrm{p}} - \mathrm{F}_1(u_1^{\mathrm{p}})\|^2_{L^2(\Gamma_2)} \Big)$$

- Introduction of port-to-bubble map $\Longrightarrow$ **unconstrained** optimization problem
- **Nonlinear least-squares problem**
- Methods: Gauss-Newton (or Quasi-Newton)

Archetype components

For a **reference value** of geometric parameter Q_a we define **archetype** components:

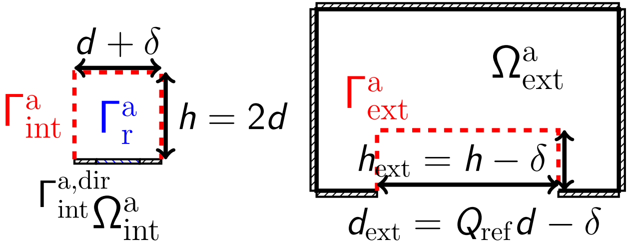


Figure 7: Archetype library $\mathcal{L}$.

Instantiated components

For any value of interest of geometric parameter $Q_{\rm a}$ we construct **instantiated** components:

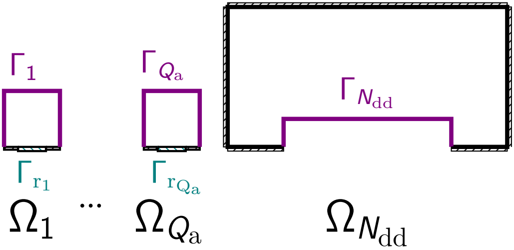


Figure 8: Instatiated (overlapping) subdomains ω_i

Offline/Online CB-pMOR procedure

Algorithm 2 Offline/online CB-pMOR procedure

Offline stage:

1: A library $\mathcal{L}$ of **archetype components** is defined
2: **for** $\mu \in \Xi_{\mathrm{train}} \subset \mathcal{P}$ **do**
3: Generate local ROBs and ROMs ▷ **localised training**
4: **endfor**

Online stage: for any new $\mu \in \Xi_{\mathrm{test}} \subset \mathcal{P}$

5: A **partition** $\{\Omega_i\}_{i=1}^{N_{\mathrm{dd}}}$ is **instantiated**
6: Compute the global solution u_μ ▷ **coupling of local ROMs**

MOR approximation for OS2

1. **Port reduction**
   Port spaces $\mathcal{Z}_i^p \subset \mathcal{U}_i$, $\mathcal{W}_i^p = \{\mathtt{E}_i\zeta : \zeta \in \mathcal{Z}_i^p \subset \mathcal{U}_i\} \subset \mathcal{X}_i$,
   Port ROB $W_i^{\mathrm{p}} : \mathbb{R}^m \to W_i^{\mathrm{p}}$

MOR approximation for OS2

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   Port spaces $\mathcal{Z}_i^p \subset \mathcal{U}_i$, $\mathcal{W}_i^p = \{\mathtt{E}_i\zeta : \zeta \in \mathcal{Z}_i^p \subset \mathcal{U}_i\} \subset \mathcal{X}_i$,
   Port ROB $W_i^{\mathrm{p}} : \mathbb{R}^m \to W_i^{\mathrm{p}}$
2. **Reduction of local maps**
   Approximate port-to-bubble map $\widehat{\mathtt{F}}_i : \mathbb{R}^m \to \mathbb{R}^n$ is s.t.

$$\widehat{\mathbf{R}}_i\left(\widehat{\mathtt{F}}_i(\boldsymbol{\beta}_i), \boldsymbol{\beta}_i\right) = 0$$

   where local residuals $\widehat{\mathbf{R}}_i : \mathbb{R}^n \times \mathbb{R}^m \to \mathbb{R}^n$ are s.t.

$$\left(\widehat{\mathbf{R}}_i(\boldsymbol{\alpha}, \boldsymbol{\beta})\right)_j = \mathcal{G}_i(\hat{u}_i(\boldsymbol{\alpha}, \boldsymbol{\beta}), \zeta_{i,j}^{\mathrm{b}}),\ i = 1, 2,\ j = 1, \ldots, n$$

MOR approximation for OS2

1. **Port reduction**
   Port spaces $\mathcal{Z}_i^p \subset \mathcal{U}_i$, $\mathcal{W}_i^p = \{\mathrm{E}_i\zeta : \zeta \in \mathcal{Z}_i^p \subset \mathcal{U}_i\} \subset \mathcal{X}_i$,
   Port ROB $W_i^{\mathrm{p}} : \mathbb{R}^m \to W_i^{\mathrm{p}}$
2. **Reduction of local maps**
   Approximate port-to-bubble map $\widehat{\mathrm{F}}_i : \mathbb{R}^m \to \mathbb{R}^n$ is s.t.

$$\widehat{\mathbf{R}}_i\left(\widehat{\mathrm{F}}_i(\boldsymbol{\beta}_i), \boldsymbol{\beta}_i\right) = 0$$

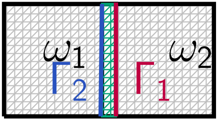
where local residuals $\widehat{\mathbf{R}}_i : \mathbb{R}^n \times \mathbb{R}^m \to \mathbb{R}^n$ are s.t.

$$\left(\widehat{\mathbf{R}}_i(\boldsymbol{\alpha}, \boldsymbol{\beta})\right)_j = \mathcal{G}_i(\hat{u}_i(\boldsymbol{\alpha}, \boldsymbol{\beta}), \zeta_{i,j}^{\mathrm{b}}),\ i = 1, 2,\ j = 1, \dots, n$$

$$\hat{u}_i(\boldsymbol{\alpha}_i, \boldsymbol{\beta}_i) = Z_i^b \boldsymbol{\alpha}_i + W_i^{\mathrm{p}} \boldsymbol{\beta}_i, \quad i = 1, 2$$

ROM OS2 formulation

Find $\widehat{\boldsymbol{\beta}} = [\widehat{\boldsymbol{\beta}}_1, \widehat{\boldsymbol{\beta}}_2] \in \mathbb{R}^{M:=2m}$ such that



ROM OS2 unconstrained statement

$$\widehat{\boldsymbol{\beta}} \in \arg\min_{\boldsymbol{\beta}\in\mathbb{R}^M} \frac{1}{2}\Big(\| Z_1^{\mathrm{b}}\widehat{\mathrm{F}}_1(\boldsymbol{\beta}_1) + W_1^{\mathrm{p}}\boldsymbol{\beta}_1 - Z_2^{\mathrm{b}}\widehat{\mathrm{F}}_2(\boldsymbol{\beta}_2) - W_2^{\mathrm{p}}\boldsymbol{\beta}_2 \|^2_{L^2(\Gamma_{1,2})} +$$

$$\| Z_2^{\mathrm{b}}\widehat{\mathrm{F}}_2(\boldsymbol{\beta}_2) + W_2^{\mathrm{p}}\boldsymbol{\beta}_2 - Z_1^{\mathrm{b}}\widehat{\mathrm{F}}_1(\boldsymbol{\beta}_1) - W_1^{\mathrm{p}}\boldsymbol{\beta}_1 \|^2_{L^2(\Gamma_{2,1})} \Big)$$

13

[13] To simplify notation, $n_1 = n_2 = n$, $m_1 = m_2 = m$.

Hyper-reduced formulation

Objectives:

1. speed up assembling of **local ROMs**
2. speed up evaluation of the **objective function**

Methods:

1. **element-wise empirical quadrature (EQ)** procedure
2. EQ,variant of **empirical interpolation method (EIM)** ([14])

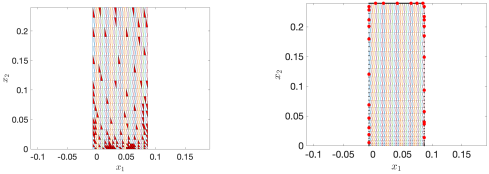


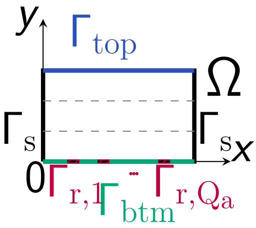
Figure 9: Sampled elements and port quadrature points in a component.

[14]Barrault et al.,C.R.M., 2004

Case study: nonlinear (neo-Hookean) elasticity

$$\begin{cases} -\nabla \cdot P(F(u)) = 0 & \text{in } \Omega \\ u \cdot \mathbf{n} = 0 & \text{on } \Gamma_{\mathrm{s}} \\ P(F(u))\mathbf{n} = g_{\mathrm{r}} = [0,\ -s]^T & \text{on } \Gamma_{\mathrm{r}} \\ P(u)\mathbf{n} = g_{\mathrm{top}} = [0,\ 4(x-1/2)(x+1/2)]^T & \text{on } \Gamma_{\mathrm{top}} \\ u = 0 & \text{on } \Gamma_{\mathrm{btm}} \end{cases}$$

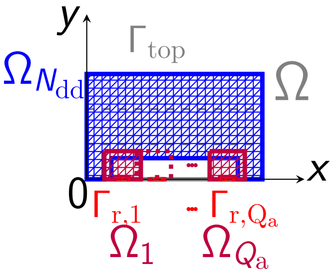
$$P(u) = \lambda_2 \left(F(u) - F(u)^{-T}\right) + \lambda_1 \log\left(\det(F(u))\right) F(u)^{-T}$$



Case study

Parameters distributions

$$(E_1, E_2, E_3, s) \overset{\text{iid}}{\sim} \text{Uniform}\left([25, 30] \times [10, 20]^2 \times [0.4, 1]\right),$$
$$Q_{\text{a}} \overset{\text{iid}}{\sim} \text{Uniform}\left(\{2, \dots, 7\}\right)$$



Training global parameters $\Xi_{\text{train}} = \{\mu^{(k)}\}_{k=1}^{n_{\text{train}}}$, $n_{\text{train}} = 70$

Out-of-sample global parameters $\Xi_{\text{test}} = \{\widetilde{\mu}^{(j)}\}_{j=1}^{n_{\text{test}}}$, $n_{\text{test}} = 20$

Numerical setting

- **Out-of-sample average prediction error**

$$E_{\rm avg} := \frac{1}{n_{\rm test}} \sum_{\mu \in \Xi_{\rm test}} \frac{\| \mathrm{P}_{\rm pu}[u_\mu^{\rm hf}] - \mathrm{P}_{\rm pu}[\widehat{u}_\mu] \|_{H^1(\Omega)}}{\| \mathrm{P}_{\rm pu}[u_\mu^{\rm hf}] \|_{H^1(\Omega)}}.$$

where $\mathrm{P}_{\rm pu}[u] := \sum_{i=1}^{N_{\rm dd}} \phi_i \, u_i \in H^1(\Omega)$ is the **partition of unity operator**.

- P2 FE discretization with $N_{\rm int}^{\rm e} = 1120$ and $N_{\rm ext}^{\rm e} = 3960$ elements.

ROM OS2: hyper-reduction

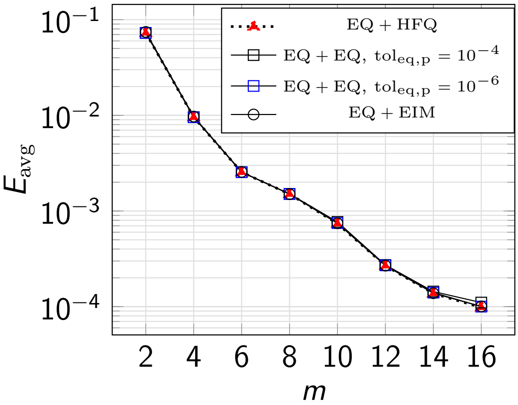


Figure 10: EIM and EQ. EQ tolerance $tol_{eq} = 10^{-10}$ for local problems and $tol_{eq,p} = 10^{-4}$, $tol_{eq,p} = 10^{-6}$ for o.f. (EQ+EQ).

ROM OS2: speedup

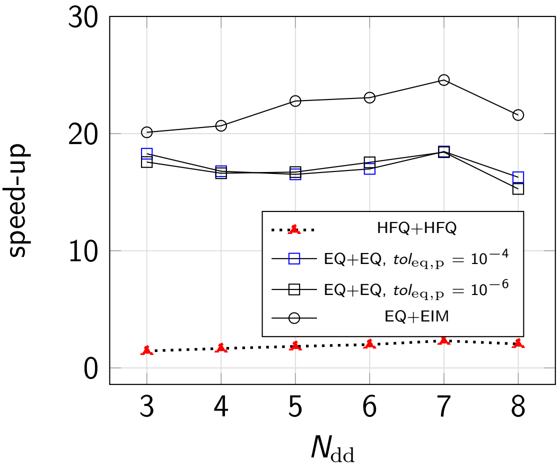
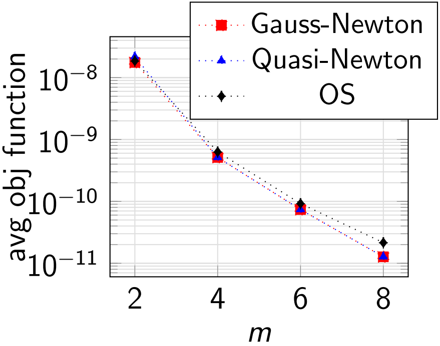
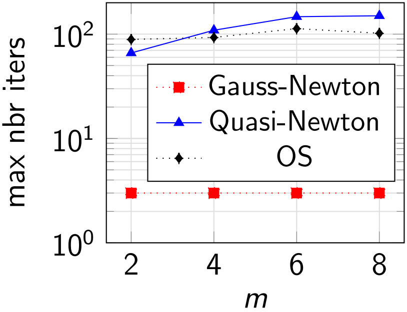


Figure 11: speedup(N_{dd}) $:= \frac{t_{\mathrm{hf(N_{dd})}}}{t_{\mathrm{OS2}}(N_{\mathrm{dd}})}$; we set $m = n = 16$, EQ tolerance $tol_{\mathrm{eq}} = 10^{-10}$.

Optimization strategy



(a) scheme convergence: objective function



(b) scheme convergence: iterations

Figure 12: comparison between OS2 with Gauss-Newton, quasi-Newton, OS.

Formulation

Given $\mu = (\mu_1, \mu_2) \in \mathcal{P} = \bigotimes_{i=1}^{2} \mathcal{P}^i$, find $\overrightarrow{\underline{\mathbb{U}}} = \{\underline{\mathbb{U}}_1, \underline{\mathbb{U}}_2\} \subset \mathcal{X}$, with $\mathcal{X} = \bigotimes_{i=1}^{2} \mathcal{X}_i$ that solves for $j = 1, \dots, J_{\max}$

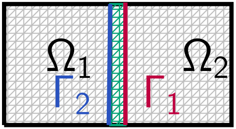
Constrained optimization statement

$$\min_{\underline{U}^{(j)} \in \mathcal{X}} \frac{1}{2} \left(\| \underline{U}_1^{(j)} - \underline{U}_2^{(j)} \|^2_{L^2(\Gamma_1)} + \| \underline{U}_2^{(j)} - \underline{U}_1^{(j)} \|^2_{L^2(\Gamma_2)} \right)$$

$$\text{s.t.}$$

$$\mathcal{G}_1^{(j)}(\underline{U}_1^{(j)}, \underline{V}_1) = 0 \quad \forall\, \underline{V}_1 \in \mathcal{X}_{1,0},$$

$$\mathcal{G}_2^{(j)}(\underline{U}_2^{(j)}, \underline{V}_2) = 0 \quad \forall\, \underline{V}_2 \in \mathcal{X}_{2,0}$$



Formulation

Given $\mu = (\mu_1, \mu_2) \in \mathcal{P} = \bigotimes_{i=1}^{2} \mathcal{P}^i$, find $\overrightarrow{\underline{\mathbb{U}}} = \{\underline{\mathbb{U}}_1, \underline{\mathbb{U}}_2\} \subset \mathcal{X}$, with $\mathcal{X} = \bigotimes_{i=1}^{2} \mathcal{X}_i$ that solves for $j = 1, \ldots, J_{\max}$

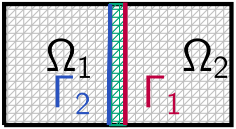
Constrained optimization statement

$$\min_{\underline{U}^{(j)} \in \mathcal{X}} \frac{1}{2} \left(\|\underline{U}_1^{(j)} - \underline{U}_2^{(j)}\|_{L^2(\Gamma_1)}^2 + \|\underline{U}_2^{(j)} - \underline{U}_1^{(j)}\|_{L^2(\Gamma_2)}^2 \right)$$

$$\text{s.t.}$$

$$\mathcal{G}_1^{(j)}(\underline{U}_1^{(j)}, \underline{V}_1) = 0 \ \ \forall\, \underline{V}_1 \in \mathcal{X}_{1,0},$$

$$\mathcal{G}_2^{(j)}(\underline{U}_2^{(j)}, \underline{V}_2) = 0 \ \ \forall\, \underline{V}_2 \in \mathcal{X}_{2,0}$$



where internal variables only enter the constraints:

$$\mathcal{G}_i^{(j)}(\underline{U}_i^{(j)}, \underline{V}) = \mathcal{G}_i(\underline{U}_i^{(j)}, \underline{U}_i^{(j-1)}, \underline{W}_i^{(j)}, \underline{W}_i^{(j-1)}, \underline{V}; \mu_i).$$

Solution to the OS2 formulation

- **Unconstrained** fomulation for each time step;
- **adaptation** of the training phase, Gauss-Newton's procedure, hyper-reduction to
  - **time-dependendency**;
  - presence of **internal** variables.

Parameters distributions:

$$\left(E_1^{(k)}, \mu_1^{(k)}, C_{\mathrm{al}}^{(k)}, \tau^{(k)}\right) \overset{\mathrm{iid}}{\sim} \mathcal{U}\big([928.14, 1.09 \cdot 10^3] \times [0.28, 0.32] \times [4.91, 5.76] \times [0.42, 0.49]\big),$$

$$Q_{\mathrm{a}} \overset{\mathrm{iid}}{\sim} \mathrm{Uniform}\big(\{2, \ldots, 7\}\big).$$

Numerical setting

- $n_{\mathrm{test}} = 5$,
- $\mathtt{I}_{\mathrm{s}} \subset \{1, \dots, J_{\max}\}$ with $|\mathtt{I}_{\mathrm{s}}| = 20$,
- $\Delta t = 0.05$.

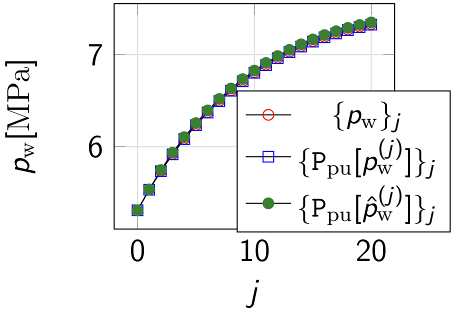
To assemble together the solutions, we use the **partition of unity operator** $\mathtt{P}_{\mathrm{pu}}[u] := \sum_{i=1}^{N_{\mathrm{dd}}} \phi_i \, u_i \in H^1(\Omega)$.

Out-of-sample prediction error:

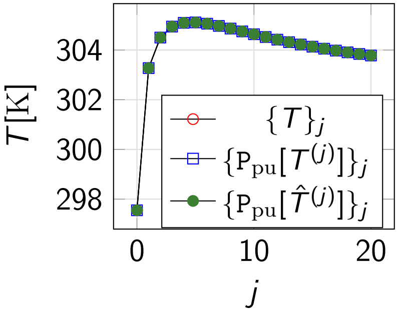
$$E_J := \frac{1}{n_{\mathrm{test}}} \sum_{\mu \in \Xi_{\mathrm{test}}} \frac{\sqrt{\sum_{j=1}^{J_{\max}} (t^{(j)} - t^{(j-1)}) \left\| \mathtt{P}_{\mathrm{pu}}[\underline{U}^{(j)}] - \mathtt{P}_{\mathrm{pu}}[\underline{\widehat{U}}^{(j)}] \right\|_{H^1(\Omega)}^2}}{\sqrt{\sum_{j=1}^{J_{\max}} (t^{(j)} - t^{(j-1)}) \left\| \mathtt{P}_{\mathrm{pu}}[\underline{U}^{(j)}] \right\|_{H^1(\Omega)}^2}}$$

to compare with the best-fit error.

OS2 without hyper-reduction



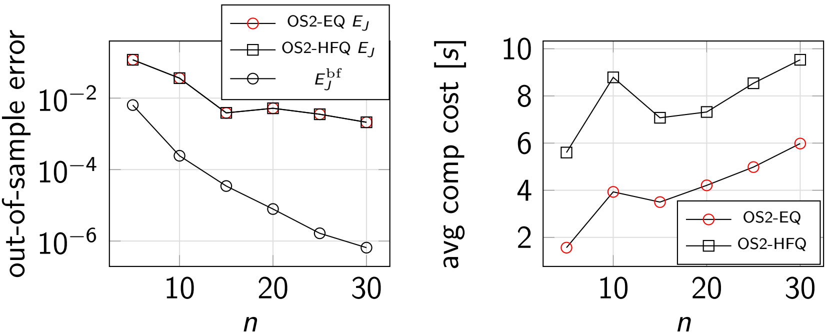
(a) pressure evolution



(b) temperature evolution

Figure 13: Two dimensional solutions in time for $\mu = \bar{\mu}$, found by global solve, by HF OS2 and by ROM hyper-reduced OS2 for $m = 40$, $n = m$.

Hyper-reduced OS2



(a) error (b) avg computational cost

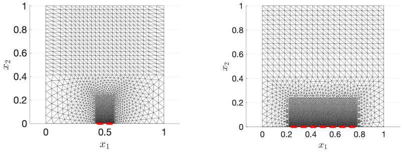
Figure 14: Performance of hyper-reduced OS2 with $tol_{\mathrm{eq}} = 10^{-14}$.

Speedup factor: $13 - 22$ for $n \in \{15, 20, 25, 30\}$ and $m = n$.

Conclusions

We developed **CB-pMOR methods** in radioactive waste applications.

1. Query costs reduction for **nonlinear mechanics** problems with **internal variables**;
2. Variation in **geometric parameters**



- by a new one-shot overlapping Schwarz (OS2) method for steady elliptic PDEs;
- by the extension of OS2 to coupled problems with internal variables.

Perspectives

- Extension to **different dimensions** of reduced bases in different archetype components;
- numerical investigation on **scaling** techniques in the OS2 objective function;
- **localized training**: extension of [15] to unsteady PDEs with internal variables;
- combination of our approach with **OS method** in [16] for time-dependent problems;
- combination of projection-based ROM and **data-fitted** methods in OS2 formulation.

[15] Smetana, Taddei, arXiv preprint arXiv:2202.09872, 2022.

[16] Mota, Tezaur, Philpot, IJNME, 2022.

Thank you for your attention!

The THM model

Physical assumptions:

- fully-saturated-in-liquid **porous medium**,
- small displacements,
- no chemical reactions.

Coupling of three phenomena: **mechanics**, **hydraulics** and **heat transfer**.

State variables $\underline{U} = [\underline{u}^{\mathrm{T}}, p_{\mathrm{w}}, T]^{\mathrm{T}}$

	SI unit	description
$\underline{u}$	m	solid displacement
p_{w}	Pa	water pressure
T	K	temperature

Table 1: state variables

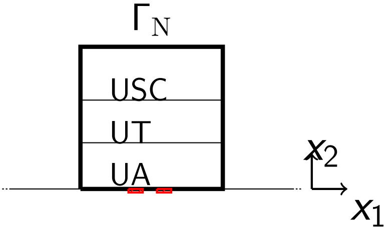
Fundamental definitions

Internal variables $\underline{W} = [\rho_\mathrm{w}, \varphi, h_\mathrm{w}, Q, \underline{M}_\mathrm{w}^\mathrm{T}, m_\mathrm{w}]^\mathrm{T}$.

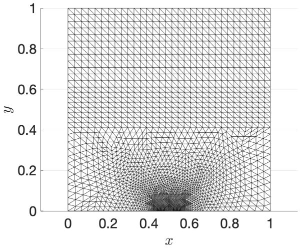
	SI unit	label
ρ_w	$\mathrm{kg} \cdot \mathrm{m}^{-3}$	water density
φ	%	Eulerian porosity
h_w	$\mathrm{J} \cdot \mathrm{Kg}^{-1}$	mass enthalpy of water
$\mathcal{Q}$	Pa	non-convected heat
$\underline{M}_\mathrm{w}$	$\mathrm{kg} \cdot \mathrm{m}^{-2} \cdot \mathrm{s}^{-1}$	mass flux
m_w	$\mathrm{kg} \cdot \mathrm{m}^{-3}$	mass input

Table 2: internal variables

Geometry configurations



(a)



(b)

Figure 15: geometric configuration: (a) the non-dimensional domain, (b): the mesh $\mathcal{T}_1$.

Mechanics

$$\begin{cases} -\nabla \cdot \underline{\underline{\sigma}} \;=\; \rho \underline{F}_{\mathrm{m}} & \text{in}\, \Omega, \\ \underline{\underline{\sigma}}\, \underline{n} = \underline{g}_{\mathrm{m,N}} & \text{on}\, \Gamma_{\mathrm{N}} = \underline{e}_2, \\ \underline{u} \cdot \underline{n} = 0 & \text{on}\, \partial\Omega \setminus \Gamma_{\mathrm{N}}, \\ (\underline{\underline{\sigma}}\, \underline{n}) \cdot \underline{t} = 0 & \text{on}\, \partial\Omega \setminus \Gamma_{\mathrm{N}}, \end{cases}$$

where the Cauchy stress tensor is

$$\begin{aligned} \underline{\underline{\sigma}} &= 2\mu' \underline{\underline{\epsilon}} + \lambda \mathrm{tr}(\underline{\underline{\epsilon}}) \mathbb{1} - (2\mu + 3\lambda)\alpha_{\mathrm{s}} \Delta \mathrm{T} \mathbb{1} \\ &= 2\mu' \nabla_{\mathrm{s}} \underline{u} + (\lambda\, \nabla \cdot \underline{u} \,-\, (2\mu + 3\lambda)\alpha_{\mathrm{s}} \Delta\, T)\, \mathbb{1}, \end{aligned}$$

the volumetric deformation is $\underline{\underline{\epsilon}} = \nabla_{\mathrm{s}} \underline{u} = \frac{1}{2}\left(\nabla \underline{u} + \nabla \underline{u}^T\right)$ and $\underline{F}_{\mathrm{m}} = -\frac{g}{\gamma} \underline{e}_2$.

Hydraulics

$$\begin{cases} \partial_t \, m_{\mathrm{w}} \; + \; \nabla \cdot \underline{M}_{\mathrm{w}} = 0 & \text{in}\, \Omega \\ \underline{M}_{\mathrm{w}} \cdot \underline{n} = 0 & \text{on}\, \partial\Omega \end{cases}$$

coupled to mechanical problem by the Darcy constitutive law

$$m_{\mathrm{w}} = \rho_{\mathrm{w}}(1 + \epsilon_{\mathrm{V}})\, \varphi - \rho_{\mathrm{w}}^0 \varphi^0,$$

with

$$\underline{M}_{\mathrm{w}} = -\gamma\, (\nabla p_{\mathrm{w}} - \rho_{\mathrm{w}} \underline{F}_{\mathrm{m}}),$$

$$\gamma = \rho_{\mathrm{w}} \frac{\kappa_{\mathrm{w}}\, \sigma_0\, \bar{t}}{\rho_0 \mu_{\mathrm{w},0}\, \bar{H}^2} \exp\left(- \frac{1808.5}{T_{\mathrm{ref}} + \overline{\Delta T}\; T} \right).$$

Heat transfer

$$\begin{cases} h_{\mathrm{w}} \partial_t \, m_{\mathrm{w}} + \partial_t \, \mathcal{Q} + \nabla \cdot \left(h_{\mathrm{w}} \underline{M}_{\mathrm{w}} + \underline{q} \right) - \underline{M}_{\mathrm{w}} \cdot \underline{F}_{\mathrm{m}} = \Theta & \text{in } \Omega \\ \left(h_{\mathrm{w}} \underline{M}_{\mathrm{w}} + \underline{q} \right) \cdot \underline{n} = g_{\mathrm{t,N}} & \text{on } \partial\Omega \end{cases}$$

where the thermal flux and is given by the Fick law

$$\underline{q} = -\Lambda \nabla T,$$

$$g_{t,N} = \frac{P_{\mathrm{t}} n_c \bar{t}}{l_Q \bar{H}^2 \sigma_0} \exp\left(- t/\tau \right) \mathbb{1}_{\Gamma_{\mathrm{r}}} = C_{\mathrm{al}} \exp\left(- t/\tau \right) \mathbb{1}_{\Gamma_{\mathrm{r}}}.$$

Constitutive laws

$$
\begin{cases}
\dfrac{d\rho_{\mathrm{w}}}{\rho_{\mathrm{w}}} = \dfrac{dp_{\mathrm{w}}}{K_{\mathrm{w}}} - 3\alpha_{\mathrm{w}} dT, \\
\dfrac{d\varphi}{b - \varphi} = d\epsilon_{\mathrm{V}} - 3\alpha_{\mathrm{s}} dT + \dfrac{dp_{\mathrm{w}}}{K_{\mathrm{s}}}, \\
dh_{\mathrm{w}} = C_{\mathrm{w}}^{\mathrm{p}}\, dT + (\beta_h^{\mathrm{p}} - 3\alpha_{\mathrm{w}}\, T)\dfrac{dp_{\mathrm{w}}}{\rho_{\mathrm{w}}}, \\
\delta \mathcal{Q} = \left(\beta_{\mathcal{Q}}^{\epsilon} + 3\alpha_{\mathrm{s}} K_0\, T\right)\, d\epsilon_{\mathrm{V}} - \left(\beta_{\mathcal{Q}}^{\mathrm{p}} + 3\alpha_{\mathrm{w,m}}\, T\right)\, dp_{\mathrm{w}} + C_{\epsilon}^{0}\, dT, \\
m_{\mathrm{w}} = \rho_{\mathrm{w}}(1 + \epsilon_{\mathrm{V}})\,\varphi - \rho_{\mathrm{w}}^{0}\varphi^{0}.
\end{cases}
$$

Initial conditions

- **Deactivated repository assumptions**: $T_0 = T_{\mathrm{ref}}$, $g_{\mathrm{t,N}} = 0$
- Simplified **hydraulic equilibrium equation**

$$p_{\mathrm{w},0}(x, y) = p_{\mathrm{w,top}} + \rho_{\mathrm{w},0} g (1 - y)$$

- Simplified equilibrium equation of **mechanical forces**:

$$\int_{\Omega_i} 2\mu' \nabla_{\mathrm{s}} \underline{u}_0 : \nabla_{\mathrm{s}} \underline{v} + \lambda (\nabla \cdot \underline{u}_0)(\nabla \cdot \underline{v}) - b p_{\mathrm{w},0} \nabla \cdot \underline{v} - \rho^0 \underline{F}_{\mathrm{m}} \cdot \underline{v} \, dx = \int_{\Gamma_{\mathrm{N_i}}} \underline{g}_{\mathrm{m,N}} \cdot \underline{v} \, dx$$

for all $v \in \mathcal{X}_u$ such that $(\underline{v} \cdot \underline{n})|_{\partial\Omega_i \setminus \Gamma_N} = 0$.

- $\rho_{w,0} = 10^3 \, [\mathrm{Kg} \cdot \mathrm{m}^{-3}]$, $\rho^0 = [2450, 2450, 2500] \, [\mathrm{Kg} \cdot \mathrm{m}^{-3}]$

POD-Greedy

Algorithm 3 POD-Greedy

Require: $\Xi_{\text{train}} = \{\mu^{(k)}\}_{k=1}^{n_{\text{train}}}$, tol_{loop}, tol_{pod}, $N_{\text{count,max}}$.

$\mathcal{Z} = \emptyset$, $\boldsymbol{\lambda} = \emptyset$, $\mu^\star = \mu^{(1)}$.
for $n_{\text{count}} = 1, \ldots, N_{\text{count,max}}$ **do**
    Compute hf snapshots $\mathbb{U}_{\mu^\star}$
    $[\mathbf{Z},\ \boldsymbol{\lambda}] = \texttt{data-compression}(Z,\ \boldsymbol{\lambda}, \{\mathbb{U}_{\mu^\star}\}, (\cdot,\cdot), tol_{\text{pod}})$;
    Construct the ROM with error indicator.
    for $j = 1 : n_{\text{train}}$ **do**
        Solve the ROM for $\mu = \mu^{(k)}$ and compute Δ_μ.
    end for
    $\mu^\star = \arg\max_{\mu \in \Xi_{\text{train}}} \Delta_\mu$ ▷ Greedy search
    if $\Delta_{\mu^\star} < tol_{\text{loop}}$ **then**, ▷ Termination condition
        `break`,
    end if.
end for
    return Z and $\mu \in \mathcal{P} \mapsto \{\widehat{\boldsymbol{\alpha}_\mu}^{(j)}\}_{j=1}^{J_{\max}}$.

Solution to the OS2 minimization problem

$$f(\boldsymbol{\beta}) = \frac{1}{2}\|\mathbf{r}(\boldsymbol{\beta})\|_2^2, \quad \text{where } \mathbf{r}(\boldsymbol{\beta}) = \mathbf{P}\,\widehat{\mathrm{F}}(\boldsymbol{\beta}) + \mathbf{Q}\boldsymbol{\beta}. \tag{1}$$

for suitable matrices $\mathbf{P}$ and $\mathbf{Q}$.

$$\nabla r = \mathbf{P}\widehat{\mathbf{J}}_{\mathrm{F}} + \mathbf{Q}, \quad \nabla f = \left(\mathbf{P}\widehat{\mathbf{J}}_{\mathrm{F}} + \mathbf{Q}\right)^T r. \tag{2}$$

where

$$\widehat{\mathbf{J}}_{\mathrm{F}}(\boldsymbol{\beta}) = \mathrm{diag}\left[\widehat{\mathbf{J}}_{\mathrm{F}_1}(\boldsymbol{\beta}_1), \ldots, \widehat{\mathbf{J}}_{\mathrm{F}_{N_{\mathrm{dd}}}}(\boldsymbol{\beta}_{N_{\mathrm{dd}}})\right],$$

$$\widehat{\mathbf{J}}_{\mathrm{F}_i}(\boldsymbol{\beta}_i) := -\left(\partial_{\boldsymbol{\alpha}_i}\widehat{\mathbf{R}}_i\right)^{-1}\partial_{\boldsymbol{\beta}_i}\widehat{\mathbf{R}}_i\Big|_{(\boldsymbol{\alpha}_i,\boldsymbol{\beta}_i)=(\widehat{\mathrm{F}}_i(\boldsymbol{\beta}_i),\boldsymbol{\beta}_i)}.$$

Solution to the OS2 minimization problem

Steepest-descent or Quasi-Newton

- explicit calculation of f, ∇f
- no need of explicitly assembling $\widehat{\mathbf{J}}_{\mathrm{F}}$

Gauss-Newton

- method of choice
- need of assembling $\widehat{\mathbf{J}}_{\mathrm{F}}$ at each iteration

$$\widehat{\boldsymbol{\beta}}^{(k+1)} = \widehat{\boldsymbol{\beta}}^{(k)} - \left(\nabla \mathbf{r}\left(\widehat{\boldsymbol{\beta}}^{(k)}\right)\right)^{\dagger} \mathbf{r}\left(\widehat{\boldsymbol{\beta}}^{(k)}\right)$$

Hyper-reduction of local problems

Weighted variational form

$$\mathcal{G}_\ell^{\rm eq}(u,v) = \sum_{k=1}^{N_\ell^{\rm e}} \rho_{\ell,k}^{\rm eq} \left(\int_{\mathtt{D}_{\ell,k}} \eta_\ell^{\rm e}(u,v)\, dx \; + \int_{\partial \mathtt{D}_{\ell,k}} \eta_\ell^{\rm f}(u,v)\, dx \right)$$

where $\boldsymbol{\rho}_\ell^{\rm eq} = [\rho_{\ell,1}^{\rm eq}, \ldots, \rho_{\ell,N_\ell^{\rm e}}^{\rm eq}]^T$ sparse vector of non-negative weights.

EQ procedure

For any $\ell \in \mathcal{L}$, find a vector $\boldsymbol{\rho}_\ell^{\rm eq} \in \mathbb{R}^{N_\ell^{\rm e}}$ such that

1. $\boldsymbol{\rho}_\ell^{\rm eq}$ is as sparse as possible
2. $\left| \sum_{k=1}^{N_\ell^{\rm e}} \rho_{\ell,k}^{\rm eq} \, |\mathtt{D}_{\ell,k}| - |\Omega_\ell^{\rm a}| \right| \ll 1$;
3. $\left| \mathbf{J}_\ell^{\rm b} (\boldsymbol{\gamma}_\ell)^{-1} \left(\widehat{\mathbf{R}}_\ell^{\rm hf}(\boldsymbol{\gamma}_\ell) \; - \; \widehat{\mathbf{R}}_\ell^{\rm eq}(\boldsymbol{\gamma}_\ell) \right) \right| \ll 1$ where $\mathbf{J}_\ell^{\rm b} := \partial_{\boldsymbol{\alpha}} \widehat{\mathbf{R}}_\ell^{\rm hf}$, $\forall\, \boldsymbol{\gamma}_\ell = (\boldsymbol{\alpha}_\ell, \boldsymbol{\beta}_\ell, \mu_\ell) \in \Sigma_\ell^{\rm train, eq}$.

Hyper-reduction of local problems

Sparse representation problem

$$\min_{\boldsymbol{\rho}\in\mathbb{R}^{N_\ell^{\mathrm{e}}}} \|\boldsymbol{\rho}\|_{\ell^0}, \quad \text{s. t.} \quad \|\mathbf{C}_\ell\left(\boldsymbol{\rho}_\ell^{\mathrm{hf}} - \boldsymbol{\rho}_\ell^{\mathrm{eq}}\right)\|_2 \leq tol_{\mathrm{eq}}, \qquad (3)$$

- Problem (3) is **NP hard**.
- Approximation: **non-negative least-square problem**

Hyper-reduction of the objective function

The objective function can be written as

$$\frac{1}{2}\sum_{i=1}^{N_{\mathrm{dd}}}\sum_{j\in\mathrm{Neigh}_i}\int_{\Gamma_{i,j}}\|\widehat{u}_i(\boldsymbol{\alpha}_i,\boldsymbol{\beta}_i)-\widehat{u}_j(\boldsymbol{\alpha}_j,\boldsymbol{\beta}_j)\|_2^2\,dx \approx \frac{1}{2}\sum_{i=1}^{N_{\mathrm{dd}}}\boldsymbol{\rho}^{\mathrm{p}}_{\mathrm{L}_i}\cdot\boldsymbol{\eta}^{\mathrm{p}}_i(\boldsymbol{\alpha},\boldsymbol{\beta}) \tag{4}$$

We replace integral form in (4) with the discrete sum

$$\frac{1}{2}\sum_{i=1}^{N_{\mathrm{dd}}}\sum_{j\in\mathrm{Neigh}_i}\int_{\Gamma_{i,j}}\|\widehat{u}_i(\boldsymbol{\alpha}_i,\boldsymbol{\beta}_i)-\widehat{u}_j(\boldsymbol{\alpha}_j,\boldsymbol{\beta}_j)\|_2^2\,dx \approx \frac{1}{2}\sum_{q\in\mathtt{I}_\ell^{\mathrm{p,eq}}}(\boldsymbol{\eta}^{\mathrm{p}}_i(\boldsymbol{\alpha},\boldsymbol{\beta},\mu) \tag{5}$$

EIM

Objective: find the quadrature indices $\mathtt{I}_\ell^{\mathrm{p,eq}}\subset\{1,\ldots,N_\ell^p\}$

Hyper-reduction of the objective function

Algorithm 4 Empirical Interpolation Method for vector-valued fields

Input: $\{\psi^{\mathrm{a,p}}_{\ell,i}\}_{i=1}^{m}$, $\ell \in \mathcal{L}$

Output: $\mathtt{I}_{\ell}^{\mathrm{p,eq}} = \{\mathtt{i}^\star_{\ell,1}, \ldots, \mathtt{i}^\star_{\ell,m}\}$

Set $\mathtt{i}^\star_{\ell,1} := \arg \max_{j \in \{1,\ldots,N_\ell^{\mathrm{p}}\}} \|\psi^{\mathrm{a,p}}_{\ell,1}(x^{\mathrm{p}}_{\ell,j})\|_2$, and define $\mathcal{I}_{\ell,1} := \mathcal{I}\left(\cdot; \{\mathtt{i}^\star_{\ell,1}\}, \mathrm{span}\{\psi^{\mathrm{a,p}}_{\ell,1}\}\right)$

for $m' = 2, \ldots, m$ **do**

  Compute $r_{m'} = \psi^{\mathrm{a,p}}_{\ell,m'} - \mathcal{I}_{\ell,m'-1}\left(\psi^{\mathrm{a,p}}_{\ell,m'}\right)$

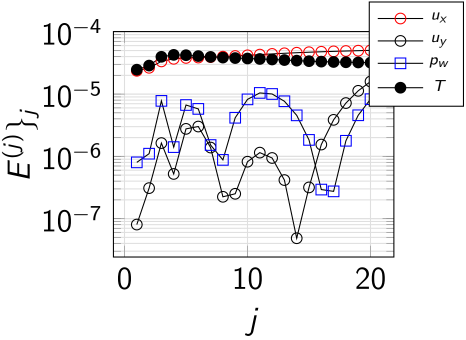
  Set $\mathtt{i}^\star_{\ell,m'} := \arg \max_{j \in \{1,\ldots,N_\ell^{\mathrm{p}}\}} \|r_{m'}(x^{\mathrm{p}}_{\ell,j})\|_2$

  Update $\mathcal{I}_{\ell,m'} := \mathcal{I}\left(\cdot; \{\mathtt{i}^\star_{\ell,j}\}_{j=1}^{m'}, \mathrm{span}\{\psi^{\mathrm{a,p}}_{\ell,j}\}_{j=1}^{m'}\right)$.

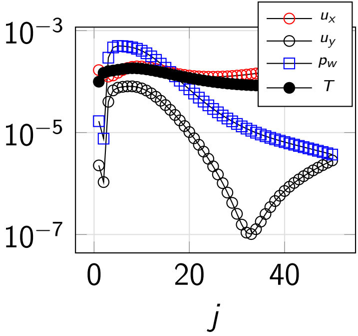
end for

Further tests

OS2-ROM without hyper-reduction for the THM system



(a) $\Delta t = 0.05$



(b) $\Delta t = 0.02$

Figure 16: $E^{(j)}\}_j$ with respect to time steps $j = 1, \ldots, J_{\max} = \frac{T_f}{\Delta t}$. Bubble and port modes are $m = n = 15$.

Further tests on OS2-ROM

OS2-ROM without hyper-reduction for the THM system

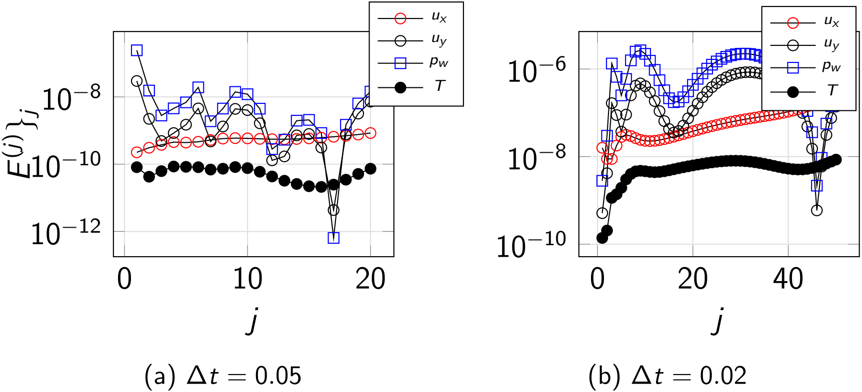


Figure 17: $E^{(j)}\}_j$ with respect to time steps $j = 1, \ldots, J_{\max} = \frac{T_f}{\Delta t}$.
Bubble and port modes are $m = n = 30$.

Further tests on OS2-ROM

OS2-ROM without hyper-reduction for the THM system

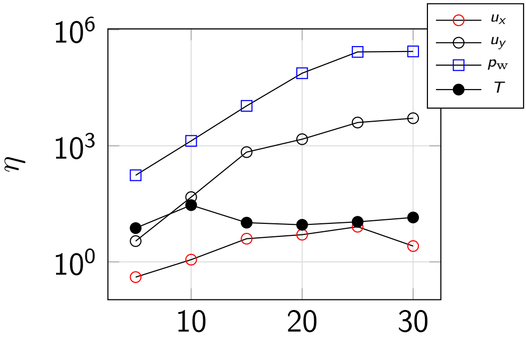


Figure 18: Efficiency ratio $\eta = \sqrt{\frac{\sum_j \|U^{(j)} - \widehat{U}^{(j)}\|^2 \Delta t}{\sum_j \inf_{\zeta \in \mathcal{Z}} \|U^{(j)} - \zeta\|^2 \Delta t}}$ for each subsolution $u_x, u_y, p_{\mathrm{w}}, T$ in a in-sample configuration.

Further tests on OS2-ROM

Study the performance of OS and OS2 with respect to overlapping size δ.

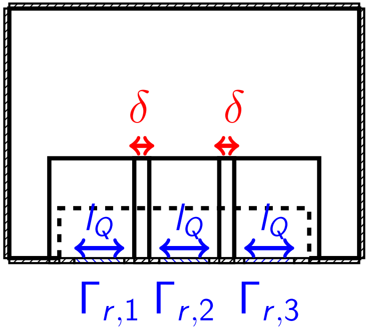


Figure 19: Example of geometric overlapping instantiated configuration for $Q_{\mathrm{a}} = 3$.

Further tests on OS2-ROM

OS2-ROM without hyper-reduction for the neo-Hookean model problem

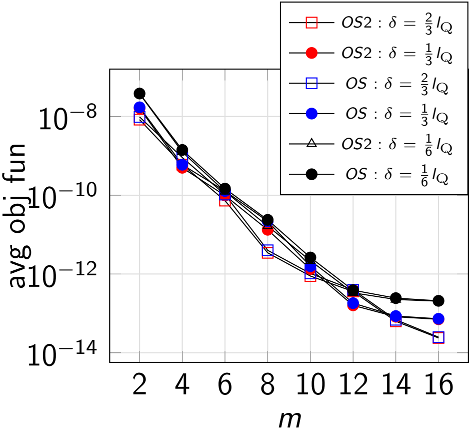


Figure 20: Out-of-sample test: OS2 and OS average values of the objective function for $\delta = \frac{2}{3} l_Q$, $\delta = \frac{1}{3} l_Q$,$\delta = \frac{1}{6} l_Q$.

Further tests on OS2-ROM

OS2-ROM without hyper-reduction for the neo-Hookean model problem

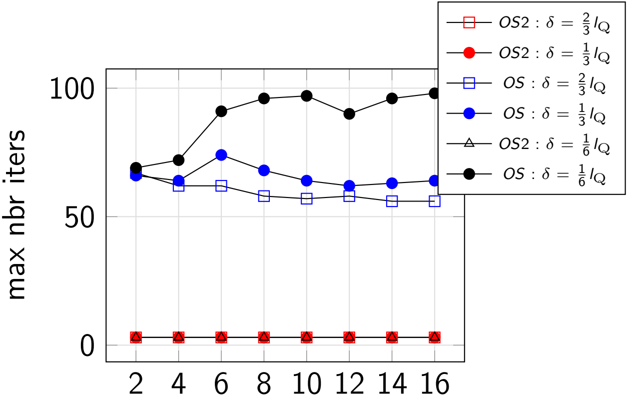


Figure 21: Out of sample test: OS2 and OS maximum numbers of iterations for $\delta = \frac{2}{3} l_{\mathrm{Q}}$, $\delta = \frac{1}{3} l_{\mathrm{Q}}$, $\delta = \frac{1}{6} l_{\mathrm{Q}}$.

Further tests on OS2-ROM

OS2-ROM without hyper-reduction for the neo-Hookean model problem

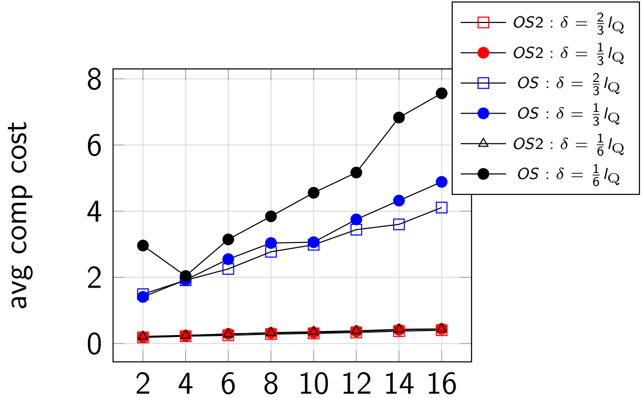


Figure 22: Out of sample test: average computational cost for $\delta = \frac{2}{3} l_Q$, $\delta = \frac{1}{3} l_Q$, $\delta = \frac{1}{6} l_Q$.